

beta-Caryophyllene
87-44-5 | DTXSID8024739

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 5.19

Global applicability domain: Inside

Local applicability domain index: 4.66e-01

Confidence level: 4.90e-01

Nearest Neighbors from the Training Set

Image not found

1-Tetradecanol

Measured: 6.03

Predicted: 6.03

Image not found

tert-Butylcyclohexane

Measured: 5.04

Predicted: 5.01

Image not found

5-Methyl-2-(propan-2-yl)cyclohexyl 2-methylbut-2-enoate

Measured: 6.20

Predicted: 5.64